Shadow Bands and Tunneling Magnetoresistance in Itinerant Electron Ferromagnets

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In itinerant electron ferromagnets spectral weight is transferred at finite temperatures from quasiparticle peaks located at majority and minority-spin band energies to shadow-band peaks. For a given Bloch wavevector and band index, the majority-spin shadow-band peak is located near the minority-spin quasiparticle energy and the minority-spin shadow-band peak is located near the majority-spin quasiparticle energy. This property can explain much of the temperature dependence seen in the magnetoresistance of magnetic tunnel junctions.

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Efforts [1] to achieve a complete understanding of late transition metal ferromagnets have been frustrated by fundamental difficulties associated with the band character of the electrons which carry the spontaneous magnetic moment. The itinerant character of magnetic electrons in these systems is incontrovertibly established by de Haas-van Alphen studies [2] which map out majority and minority spin Fermi surfaces enclosing $\vec{k}$-space volumes consistent with the measured saturation moment per atom. Nevertheless, many finite-temperature properties of these systems are inconsistent with a simple Stoner-Wolfarth [3] mean-field theory for band ferromagnets and are more easily rationalized in a picture in which the d-electrons are regarded as localized. The localized $vs.$ itinerant conundrum is often most informatively addressed by probes of the one-particle Green's function. For example, photoemission studies have [4] and continue [5] to improve insight. The present work is motivated by recent success [6] in fabricating ferromagnet-insulator-ferromagnet magnetic tunnel junctions (MTJ's) with reproducible characteristics, opening up the possibility of obtaining spin-resolved information on the tunneling density-of-states of band ferromagnets. We point out that, in an itinerant electron ferromagnet, a portion of the spectral weight is transferred at finite temperatures from a majority or minority spin quasiparticle peak to a shadow-band peak located near the opposite spin quasiparticle energy. The fraction of the spectral weight transferred is proportional, at low temperatures, to the saturation moment suppression. We propose that this effect is responsible for much [7] of the temperature-dependence of MTJ magnetoresistance (MR).

Tunneling measurements are usually interpreted by assuming a weak link which can be modeled by a phenomenological tunneling Hamiltonian. This approach allows the tunneling current to be expressed quite generally in terms of electronic spectral functions [9]. Assuming only that the temperature is much smaller than the respective band widths, the tunneling conductance between two weakly linked ferromagnets is

$$G = \frac{2\pi e^2}{\hbar} \sum_{\sigma} \sum_{n_L, \vec{k}_L} \sum_{n_R, \vec{k}_R} |t(n_L, \vec{k}_L; n_R, \vec{k}_R)|^2 \times$$
$$A^L_{n_L, \vec{k}_L, \sigma}(E_F) A^R_{n_R, \vec{k}_R, \sigma}(E_F). \tag{1}$$

Here $A_{n,\vec{k}}(E)$ is the spectral weight function for band n at wavevector $\vec{k}$, L (left) and R (right) label ferromagnets on opposite sides of the MTJ. and $\sigma = \uparrow$ (majority spin on left of junction), ($\downarrow$) (minority spin on left side of junction) labels spin. To establish notation we first discuss our view of the band theory interpretation of MTJ MR.

In band theory, metallic ferromagnets are characterized by spin-split temperature-independent energy bands with infinite quasiparticle lifetimes: $A_{n,\vec{k},\sigma}(E) = \delta(E_{n,\vec{k},\sigma} - E)$. We assume that the tunneling amplitudes appearing in Eq.(1) can be approximately decoupled into factors depending separately on band wavefunctions on opposite sides of the barrier, $i.e.$ that $|t(n_L, \vec{k}_L; n_R, \vec{k}_R)|^2 \approx |t(n_L, \vec{k}_L)||t(n_R, \vec{k}_R)|$. This assumption is physically natural and, as we comment below, is necessary to explain the common success [10] of the Jullière [11] formula in interpreting MR data. The tunneling conductance is then proportional to a sum over spin directions of the product of factors depending separately on left and right ferromagnets:

$$G = \frac{2\pi e^2}{\hbar} \sum_{\sigma} t^L_\sigma N^L_\sigma t^R_\sigma N^R_\sigma. \tag{2}$$

Here N_σ is the Fermi level density of states and t_σ is a weighted average of tunneling amplitude factors defined by

$$t_\sigma N_\sigma = \sum_{n,\vec{k}} |t_{n,\vec{k}}| \delta(E_F - E_{n,\vec{k},\sigma}). \tag{3}$$

From Eq.(2) we can evaluate the parameter usually used to characterize the size of the magnetoresistance of a MTJ:

$$MR \equiv \frac{G_P - G_A}{G_P} = \frac{2P^L P^R}{1 + P^L P^R}. \tag{4}$$

Here G_P and G_A are respectively the conductances when ordered moments on opposite sides of the junction have parallel and antiparallel orientations.

$$P = \frac{t_a N_a - t_i N_i}{t_a N_a + t_i N_i} \qquad (5)$$

where the indices a and i refer to majority and minority spins respectively. Comparing Eq.(5) and Eq.(2), P can be identified as the spin polarization of the tunneling current between a ferromagnet and a spin-unpolarized system. This quantity has been measured for most systems of interest [12]. The tunneling current is generally found to be dominated by the majority spins, even when their density of states is smaller, because tunneling amplitudes are larger [13] for states with dominant s-wave character. Eq.(4) is the Jullière [11] formula which is in good agreement with many experimental results; the present derivation demonstrates that its approximate validity rests on the factorizability of tunneling matrix elements.

We now address the importance for the MR of the modifications of band-theory which are required at finite temperatures. Up to room temperature and beyond, the main effect of finite T on late transition element ferromagnets is to excite low-energy long-wavelength spin-waves. To a good approximation, the quasiparticle bands of the ferromagnet adiabatically follow the local instantaneous orientation of the magnetic moment. Although the quasiparticle spectrum in this approximation is rigid, its projection onto the time-averaged ordered moment direction is altered. A quasiparticle whose spin is aligned with the fluctuating bands will at finite temperature be a majority spin with probability $(1 + m(T)/m_0)/2$ and a minority spin with with probability $(1 - m(T)/m_0)/2$. Here $m(T)/m_0$ is the factor by which the saturation moment is reduced at temperature T due to thermally excited spin-waves. A *shadow-band* peak must appear in the minority-spin spectral function at the majority-spin quasiparticle energy. The effect on MR of shadow-band features in the majority and minority-spin spectral functions is illustrated schematically in Fig. 1. Two terms contribute to $t_\uparrow N_\uparrow$ at finite temperatures, one arising from the majority spin quasiparticle band, the other from the minority spin shadow band. For example, in the left-ferromagnet

$$t_\uparrow^L N_\uparrow^L = \frac{1 + m(T)/m_0}{2} t_a^L N_a^L + \frac{1 - m(T)/m_0}{2} t_i^L N_i^L$$

$$t_\downarrow^L N_\downarrow^L = \frac{1 + m(T)/m_0}{2} t_i^L N_i^L + \frac{1 - m(T)/m_0}{2} t_a^L N_a^L . \quad (6)$$

Corresponding expressions apply for the right ferromagnet. It follows that the Jullière formula continues to apply at finite temperatures with a reduced polarization factor $P(T) = [m(T)/m_0] \times P(0)$ for each ferromagnet. The saturation moments, $m(T)$, of bulk late transition element ferromagnets are reduced by $\sim 5\%$ between $T = 0$ and room temperature, reduction factors are expected to be twice as large near the surface

[14], and will be larger throughout the volume of the thin film electrodes used in MTJ's. Reductions in MR exceeding $\sim 20\%$ at room temperature are therefore readily accounted for by this mechanism. It seems likely that this effect is responsible for the largest part of the MR reduction seen in experiment. An experimentally testable prediction which follows from this assertion is that [15] MR should follow a $T^{3/2}$ law at low temperatures: $MR(T) = MR(T = 0)(1 - AT^{3/2} + \ldots)$ where A is approximately the sum of the $T^{3/2}$ coefficients for the relative magnetization of the two ferromagnetic electrodes.
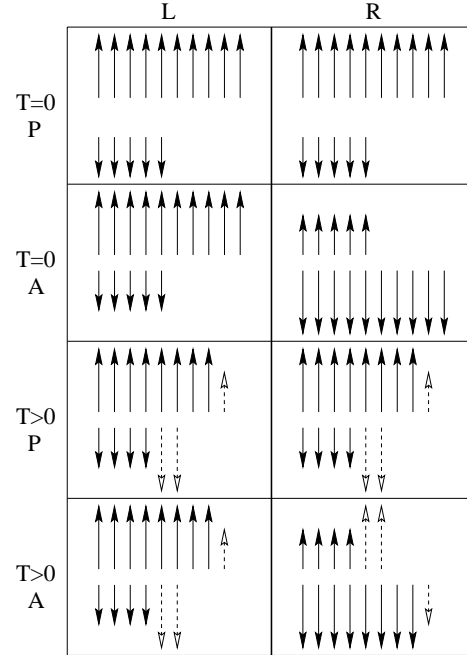

FIG. 1. Schematic illustration of spin-polarized tunneling between left (L) and right (R) ferromagnets with parallel (P) and antiparallel (A) magnetizations at zero and finite temperature. In each case long arrows represent quasiparticles whose spins are aligned with the fluctuating bands while short arrows represent quasiparticles with the opposing orientation. The number of large arrows for $T = 0$ is proportional to $t_a N_a$, and the number of small arrows proportional to $t_i N_i$. In this illustration, $t_a N_a = 10$ and $t_i N_i = 5$ in arbitrary units. At $T = 0$, $G = 10 \times 10 + 5 \times 5 = 125$ for parallel orientations, $G = 2 \times 10 \times 5 = 100$, for antiparallel orientations, and $MR = 20\%$. The finite temperature panels correspond to $m(T)/m_0 = 0.6$, so that 80% of the spectral weight resides in quasiparticle peaks (solid lines) and 20% resides in shadow-band peaks (dashed lines). The parallel orientation conductance is then reduced to $G = 9 \times 9 + 6 \times 6 = 117$,the antiparallel orientation conductance increased to $G = 2 \times 9 \times 6 = 108$, and MR decreased to 7.7%.

We now turn to a more microscopic justification for the proposed shadowband features in the electron spectral function. The abridged discussion presented here is

intended to emphasize that the effect requires only that the ground state of the ferromagnet be a spontaneously spin-polarized Fermi-liquid. It is compatible with strong local correlation features [5] being present in the spectral functions, compatible with strong band-dependence for the quasiparticle energy spin-splitting, and independent of the complexity and individuality of the quasiparticle bands of particular metallic ferromagnets. We assume that in the ground state of the ferromagnet, the one-particle Green's function is that of a spin-polarized Fermi liquid, with quasiparticle-peaks for both $\uparrow$ and $\downarrow$ spins which become arbitrarily sharp as the Fermi energy is approached:

$$[G_{n\sigma,n'\sigma'}(\vec{k},E)]^{-1} = [\delta_{n\sigma,n'\sigma'}E - H^{QP}_{n\sigma,n'\sigma'}(\vec{k},E)]^{-1}$$
$$= [\delta_{n\sigma,n'\sigma'}(E - E_{n,\sigma}(\vec{k},E)) +$$
$$i\delta_{\sigma,\sigma'}\Gamma_{n\sigma,n'\sigma}(\vec{k},E)]^{-1}. \quad (7)$$

The real part of the electronic self-energy is included in $E_{n,\sigma}(\vec{k},E)$, and we use a representation where the Green's function is diagonal in the band index n. Invariance of the system under spin-rotations about the moment direction guarantees that G is diagonal in spin-indices. At the Fermi energy, chosen as $E = 0$, the imaginary part of the self-energy, $\Gamma_{n\sigma,n'\sigma'}$, vanishes. In the most naive version of ferromagnetic band theory the quasiparticle bands are rigidly spin-split, $E_{n,\uparrow}(\vec{k},E) \rightarrow E_n(\vec{k}) - \Delta/2$ and $E_{n,\downarrow}(\vec{k},E) \rightarrow E_n(\vec{k}) + \Delta/2$. Modern spin-density functional ferromagnet quasiparticle bands are *not* rigidly spin-split, and at $T = 0$, are in rough [2,3] agreement with experiment.

In Fe, Ni, Co and their alloys it is a good approximation, up to room temperature and beyond, to account for thermal fluctuations only in the ordered moment direction, to assume that these vary slowly on an atomic length scale, and to regard the quasiparticles as separate but coupled degrees of freedom. Keeping only the leading term in a gradient expansion, the excess energy density is $\rho_s|\nabla\hat{n}|^2/2$ where $\hat{n} = (n_x, n_y, n_z)$ is the unit vector which defines the local ordered moment orientation and ρ_s is the spin-stiffness. For small tilts away from the $\hat{z}$ direction, the excess energy due to spin fluctuations, H^{SW}, may be expressed in terms of transverse components of the moment orientation vector. Fourier transforming we find that

$$H^{SW} = \frac{\rho_s}{2V}\sum_{\vec{q}} q^2 [n_{x-\vec{q}}n_{x\vec{q}} + n_{y-\vec{q}}n_{y\vec{q}}]. \quad (8)$$

The quantum commutator between transverse spin-components may be replaced by a c-number as long as the saturation moment suppression is not large:

$$[n_{x-\vec{q}}, n_{y\vec{q}'}] = i\delta_{\vec{q},\vec{q}'}\frac{2V}{m_0}. \quad (9)$$

In Eq.(9), which results from coarse graining electron spin commutation relations, V is the system volume. This leads to a free boson spin-wave Hamiltonian:

$$H^{SW} = E_0 + \sum_{\vec{q}} \epsilon_{SW}(\vec{q})\, a^{\dagger}_{\vec{q}}a_{\vec{q}}, \quad (10)$$

where $[a_{\vec{q}}, a^{\dagger}_{\vec{q}'}] = \delta_{\vec{q},\vec{q}'}$, and $\epsilon_{SW}(\vec{q}) = Dq^2 = 2\rho_s q^2/m$. The expression we use below for spin-wave quasiparticle coupling follows from the relationship between the spin-wave annihilation operator and the Fourier transforms of the transverse spin-orientation field:

$$a_{\vec{q}} = \left(\frac{m_0}{4V}\right)^{1/2}(n_{x\vec{q}} + in_{y\vec{q}}) \quad (11)$$

In the fluctuating band picture of itinerant electron ferromagnets, quasiparticle bands rotate in spin-space along with a slow variation in the ordered moment direction. At the Fermi energy the imaginary part of the quasiparticle self-energy can be neglected and

$$H^{QP}_{n\sigma,n'\sigma'}(\vec{k},E=0) \rightarrow \frac{\delta_{n,n'}}{2}(E_{n,\uparrow}(\vec{k}) + E_{n,\downarrow}(\vec{k}) -$$
$$\Delta_n(\vec{k})\,\vec{\sigma}_{\sigma,\sigma'} \cdot \hat{n}) \quad (12)$$

where $\vec{\sigma}$ are the Pauli matrices, $\Delta_n(\vec{k}) \equiv E_{n,\downarrow}(\vec{k}) - E_{n,\uparrow}(\vec{k})$ is the band and wavevector dependent spin-splitting, and all self-energies have been evaluated at $E = 0$. Expanding the right hand side of Eq.(12) to leading order in n_x and n_y, the zeroth order term gives the ground state quasiparticle bands and the leading order correction gives the spin-wave quasiparticle interaction. Allowing the orientation to vary slowly [16] in space and Fourier transforming leads to the following interaction Hamiltonian between quasiparticles and spin-waves, written in second quantized form:

$$H^{SW-QP} = \sum_{n,\vec{k},\vec{q}} \frac{\Delta_n(\vec{k})}{Vm}[c^{\dagger}_{n,\vec{k}+\vec{q}/2,\uparrow}c_{n,\vec{k}-\vec{q}/2,\downarrow}a^{\dagger}_{\vec{q}} + h.c.]$$
$$(13)$$

The evaluation of single spin-wave self-energy diagrams corresponding to H^{SW-QP} is similar to that for phonon-exchange [17] in metals and leads to:

$$\Sigma_{n\uparrow}(\vec{k},E) = \int \frac{d\vec{q}}{(2\pi)^3}\Delta_n^2(\vec{k}+\vec{q}/2) \times$$
$$\frac{n_B(\epsilon_{SW}(\vec{q})) + n_F(E_{n\downarrow}(\vec{k}+\vec{q}))}{[E + \epsilon_{SW}(\vec{q}) - E_{n\downarrow}(\vec{k}+\vec{q})]}. \quad (14)$$

Because of the gapless spin-wave excitations, the Fermi occupation factor, n_F, in the numerator of the integrand can be neglected at finite temperatures in comparison with the Bose factor, n_B. The integration is dominated by the k-space volume satisfying $\epsilon_{SW}(\vec{q}) < k_B T$. We assume that at temperatures of interest $q's$ satisfying this inequality are small compared to Brillouin-zone dimensions and set $\vec{q} \rightarrow 0$ on the right hand side of Eq.(14). These approximations lead to

$$\Sigma_{n\uparrow}(\vec{k}, E) \approx \frac{\Delta_n^2(\vec{k})}{2} \frac{1 - m(T)/m_0}{E - E_{n\downarrow}(\vec{k})}. \qquad (15)$$

where

$$\frac{m(T)}{m_0} = 1 - \frac{2}{m_0} \int \frac{d\vec{q}}{(2\pi)^3} n_B(\epsilon_{SW}(\vec{q})) \qquad (16)$$

is the relative magnetization suppression due to thermal spin-wave excitations. A similar calculation gives the contribution to the spin $\downarrow$ self-energy:

$$\Sigma_{n\downarrow}(\vec{k}, E) \approx \frac{\Delta_n^2(\vec{k})}{2} \frac{1 - m(T)/m_0}{E - E_{n\uparrow}(\vec{k})}. \qquad (17)$$

These simple self-energy expressions give Dyson equations which can be solved analytically. The spin $\uparrow$ Green's function has two simple poles, one at $E_{n\uparrow}(\vec{k})$ and one at $E_{n\downarrow}(\vec{k})$. When the magnetization suppression is small, the spectral weights of the two-poles are $(1+m(T)/m_0)/2$ and $(1-m(T)/m_0)/2$ respectively, in agreement with the naive fluctuating band argument given above. Similarly the spin $\downarrow$ Green's function splits its spectral weight between poles at the $T = 0$ minority and majority band positions. When the magnetization suppression is large, the low-temperature approximations leading to this result begin to fail and alteration of the low-temperature spectral weights will become more complex and more material specific.

Experimental progress continues to reduce the influence of unintended extrinsic effects on the properties of MTJ's. We have suggested that the temperature-dependence of the MR of MTJ's is a consequence of the formation of sharp shadowband features in the one-particle Green's function tunneling density of states. For a given band and spin index, shadow bands are located near the quasiparticle peak of the opposite spin. The occurrence of shadowbands of this type is expected in the fluctuating band picture of metallic ferromagnets. The temperature-dependence explanation in terms of intrinsic properties of bulk ferromagnets offered here, encourages the hope that MTJ tunneling spectroscopy can be developed into a probe of the single-particle Green's function of itinerant electron ferromagnets with a power similar to that of photoemission.

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[15] Below $T \sim 10K$ corrections due to the gap in the spin-wave spectrum created by anisotropy and internal fields can alter this result.

[16] For spatially constant $\hat{n}$ the interaction is diagonal in band indices and therefore non-local in space. For slowly varying $\hat{n}$ we evaluate the $\hat{n}$ at the mid-point of *bra* and *ket* position vectors. Spin-wave quasiparticle interactions which are off-diagonal in band index vanish linearly with wavevector and are taken to be negligible here.

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